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On the numerical modeling of supercooled micro-droplet impact and freezing on superhydrophobic surfaces

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ABSTRACT

Most of the ice accretion on airframe is due to supercooled droplets in clouds which are located at altitudes below 2400 m which aircrafts frequently have to pass during takeoff and landing. In the present work, the impact and freezing of a supercooled droplet on a superhydrophobic surface with hysteresis is modeled based on (i) the volume of fluid (VOF) method coupled with a dynamic contact angle model, (ii) the modified momentum and the enthalpy formulation of the energy equations for the phase change during freezing, (iii) the nucleation theory, making use of Gibbs function as an energy barrier to be overcome before the supercooled liquid instantly freezes upon contact with the substrate. The simulation retrieves the characteristic concave ice-shape during droplet freezing, which is also found to promote the contact angle pinning. The solidification time which controls the type of ice is found to evolve exponentially with the droplet maximum spreading diameter. The simulations results agree well with the experimental data of supercooled droplet from the literature. The approach developed in this paper, which accounts for droplet nucleation and freezing mechanism, can be used to model and better understand the impact of supercooled water droplets of various sizes involved in ice accretion on aircraft wings leading edge.

1. Introduction

Only in the US, airframe icing is responsible for more than 50 incidents and the loss of more than 800 lives between 1982 and 2000 [1]. Ice on aircrafts, roadways, and wind turbines are probably the most serious meteorological hazard facing the associated industries. Most of the ice accretion on airframe is due to supercooled droplets in clouds which are located at altitudes below 2400 m which aircrafts frequently have to pass during takeoff and landing. The resulting in-flight icing of supercooled liquid water (SLW) droplet can take place on aircraft wing, tail, engine or instrument and lead to decrease the aerodynamic performance which could result in a lack of control or loss of thrust and constitute a major safety and security issue. In addition to the small SLW droplets (smaller than 50 μm), the supercooled large droplets (SLD) with sizes larger than 50 μm have been the focus of many researches. Better understanding of droplet impact dynamics including spreading, splashing, and recoiling on surfaces with various wettabilities from hydrophilic to superhydrophobic is necessary to predict the ice accretion on aircraft components.

The pioneering work on droplet spreading and solidification has been carried out by Madejski in 1976 [2]. His analytical approach provides an estimation of the spreading diameter (or the degree of flattening) during solidification by combining the Stefan problem and a simple radial flow assumption. His model based on a 2D axisymmetric flow of the velocity field has been improved in [3] using a more suitable approximation for both the velocity field and the dissipation. Those works were only concerned with metal droplet solidification and do not address the water freezing. There are very few publications addressing water droplet solidification apart from the early work by Anderson et al. [4–6] based on geometrical analysis. More recently a geometrical model has been developed to analyze the singularity at the tip of a frozen water droplet [7–9]. These models neglect the droplet impact as well as the spreading; in addition, they cannot predict the concave ice-front evolution.

It is worth noting that recent experimental, theoretical, and numerical works on supercooled droplet freezing are focused on the micro-physical processes involved such as the pattern and growth of dendrite following droplet impact. The relevant parameters controlling ice dendrites growth within supercooled pure water is investigated theoretically and experimentally in [10]. A very good agreement has been found on dendrite tip velocity between the numerical simulations based on both volume of fluid

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Nomenclature

C_p	specific heat (J/K kg)
D_0	droplet initial diameter (m)
D_{max}	droplet maximum spreading diameter (m)
V_0	impact velocity (m/s)
U_{cl}	contact line velocity (m/s)
f_{ls}	liquid–solid(Ice) volume fraction
H	total enthalpy (J)
k_B	Boltzmann constant (J/K)
k_l	liquid-ice phase fraction parameter (1/K)
L	latent heat of fusion (J/kg)
P	pressure (Pa)
T	temperature (K)
g	gravitational acceleration (m/s^2)
λ	thermal conductivity (W/m K)
t	time (s)
U	velocity field (m/s)
υ_s	approximate ice volume within the droplet (m^3)
V_T	droplet total volume (m^3)
ΔG	free Gibbs energy (J)
$S(\theta_E)$	wetting parameter

α	volume of fluid fraction
θ	dynamic contact angle
ν	kinematic viscosity (m^2/s)
γ	interfacial gas–liquid surface tension (N/m)
γ_{LS}	interfacial ice-liquid surface tension (N/m)
ρ	density (kg/m^3)
τ_s	freezing time (s)

Subscripts

E	equilibrium
A	advancing
R	receding
l	liquid
s	solid (ice)

Dimensionless numbers

Ec	Eckert number ($V_0^2/C_p\Delta T$)
Re	Reynolds number ($\rho V_0 D_0/\mu$)
We	Webber number ($\rho V_0^2 D_0/\gamma$)

and level set methods, the experiments and the marginal stability theory of Langer and Müller-Krumbhaar in [11]. In addition, by repeating numerous supercooled droplets impact, a statistical model has been derived in [12] to estimate the rate of heterogeneous nucleation. A nice review in the physics, hydrodynamics and thermodynamics involved in the supercooled water droplet freezing can been found in [13]. Although essential in understanding the underlying micro-physical processes involved in supercooled droplet freezing, the modeling of dendritic ice is not enough to capture the full picture of supercooled droplet impact and freezing; and there is still a challenge to derive a numerical model, retaining the relevant physics, capable of simulating the solidification of supercooled water droplet upon impact on a solid substrate. The present work focuses on modeling the dynamics of droplet impact and freezing and can be considered as complementary to the work in [13,14] where the emphasis is on analyzing dendritic ice growth.

From a numerical point of view, for instance, the work by Pasandideh-Fard et al. [15] which relies on the enthalpy formulation in [16,17] is one of the few works reported treating droplet impact and solidification, though their approach is based on the weak formulation method and is more suited for metal droplet as pointed out by these authors. Although their approach dealt with numerical modeling of droplet impact, their model still makes use of experimental data to describe the complex dynamic contact angle for the spreading and neglect the surrounding air presence considered as void. It is important to emphasize that air may be entrapped at droplet impact and modify the heat transfer inside the droplet [18,19]. Recently in [20] under static condition, the freezing of a water droplets on hydrophobic and hydrophilic surfaces under rapid cooling condition was investigated. A single phase numerical simulation is also performed to determine the temperature field within the droplet, while the ice fraction is approximated through an energy balance equation. In [21], considering droplet dynamics, it is shown experimentally, using both infrared (IR) thermometry and high-speed imaging, the critical role played by the contact area in controlling water droplet freezing. The mechanism of supercooled water droplet freezing under the effect of airflow has been experimentally investigated in [22], and the effect of the surrounding environment in controlling ice crystallization mechanism is evidenced.

Blake et al. [23] propose an approach to perform droplet freezing, however the model relies on the classical formulation in [16,17]. In addition, the rapid phase change is not considered, the simulation are performed only after the recalescence phase. The same model has been used in [24] with the impact on inclined plane. However, this rapid growth phase is critical for droplet dynamics freezing as the nucleation and subsequent pinning occur during that phase. Zhao *et al.* [25] uses an interesting approach, based on lattice Boltzmann method (LBM), to model the impact and freezing of a saturated liquid droplet on a cryogenic spot. However, the validation with experiment is not provided. In addition, their solidification model relying on the solidus and liquidus temperatures would be more convenient for metal solidification [15]. Furthermore, the surface hysteresis effect is not considered. Unlike most of the models in the literature, the present work addresses the following challenges pertaining to supercooled droplet modeling which make it unique: (i) phase change for water at a fixed (defined) temperature, instead of assuming the freezing to occur over a range of temperature, (ii) the dynamic contact angle and hysteresis effect are accounting for in order to accurately capture droplet impact dynamics, (iii) heterogeneous nucleation which controls the pinning upon droplet impact and freezing will also be incorporated into our model.

We recently showed in [26] both theoretically and experimentally the critical role played by the surrounding air on supercooled water droplet dynamics impacting on superhydrophobic surfaces. Although the Volume of Fluid (VOF) model can capture the physics governing metal solidification phenomenon relatively well (albeit neglecting the air phase), the water freezing problem which presents much more severe discontinuity at the phase front, seems out of reach by the conventional technique based on the enthalpy formulation as pointed out in [15]. Finding a formulation for water droplet capable of addressing these limitations of the enthalpy method will be one of the aims of the present paper.

Since all the icing certification conditions are tested in flight condition and/or tunnel experiments mostly due to the cost, development of reliable numerical tools is necessary. Most of the codes for aircraft icing are based either on thin film approach, panel method, or over-simplified scenarios for droplet impact and solidification using the average mass and heat transfer balance at the surface to predict ice accretion and neglect the dynamics of droplet